**Electronic Supplementary Information (ESI)**

CO catalytic oxidation on Al-doped graphene-like ZnO monolayer sheets:

* a first-principles study

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**Fig. S1.** Several atomic configurations for the O$_2$ ((a), (b), and (c)) and CO ((d) and (e)) adsorption on the pristine g-ZnO monolayer sheet. The nearest distance between the adsorbed molecules and the sheet, and the adsorption energies are given.

(a) $E_a = 0.02$ eV  
\[d = 3.23 \text{ Å}\]

(b) $E_a = 0.02$ eV  
\[d = 3.08 \text{ Å}\]

(c) $E_a = 0.02$ eV  
\[d = 2.97 \text{ Å}\]

(d) $E_a = 0.03$ eV  
\[d = 2.91 \text{ Å}\]

(e) $E_a = 0.01$ eV  
\[d = 3.22 \text{ Å}\]

**Fig. S2.** Atomic configurations of two typical states for the O$_2$ adsorption at the sites away from the doped Al atom on the Al-g-ZnO monolayer sheet. The adsorption energies are given.

(a) $E_a = 0.86$ eV  
\[2.12 \text{ Å}, 1.39 \text{ Å}, 2.13 \text{ Å}\]

(b) $E_a = 1.15$ eV  
\[2.14 \text{ Å}, 1.39 \text{ Å}, 2.09 \text{ Å}\]
**Fig. S3.** The atomic configurations and adsorption energies for the states of O$_2$ dissociative adsorption on the Al-g-ZnO monolayer sheet. The O atoms from the dissociated O$_2$ are denoted as blue spheres. The adsorption energies were calculated with respect to the free O$_2$ molecule and the bare Al-g-ZnO sheet.

<table>
<thead>
<tr>
<th>State</th>
<th>Adsorption Energy (eV)</th>
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<tbody>
<tr>
<td>(a)</td>
<td>$E_a = 0.13$ eV</td>
</tr>
<tr>
<td>(b)</td>
<td>$E_a = 0.24$ eV</td>
</tr>
<tr>
<td>(c)</td>
<td>$E_a = 0.15$ eV</td>
</tr>
<tr>
<td>(d)</td>
<td>$E_a = 0.04$ eV</td>
</tr>
<tr>
<td>(e)</td>
<td>$E_a = 0.11$ eV</td>
</tr>
<tr>
<td>(f)</td>
<td>$E_a = 0.23$ eV</td>
</tr>
</tbody>
</table>

**Fig. S4.** Atomic configuration of the considered initial (left) and fully optimized (right) states for the coadsorption of O$_2$ and CO molecules on the Al-g-ZnO monolayer sheet.
**Fig. S5.** Atomic configuration of the carbonate-like MS state and the state of CO$_2$ physisorbed on the atomic O-covered Al-g-ZnO monolayer sheet are shown in (a) and (b), respectively. The former is more stable than the latter by 1.48 eV.